AMENDMENTS TO THE CLAIMS

1-2. (CANCELLED)

3. (CURRENTLY AMENDED) A computer-implemented method of constructing a model for predicting molecular behavior using marker molecules, said method comprising:

classifying respective molecules in a training set of reference molecules as either possessing or not possessing at least one chemical or biological property;

selecting, from said training set, a plurality of molecules that possess said at least one chemical or biological property as target molecules for potential selection as marker molecules for said model; ~~a first subset of said training set of reference molecules, wherein all of the molecules in said subset possess the at least one property~~;

selecting some of said target molecules as marker molecules for said model by evaluating the predictive accuracy of said potential marker molecules, wherein said evaluating comprises:

~~comparing all molecules in said training set with all other molecules in said training set in accordance with~~ computing a numerical value defining a measure of molecular structural similarity for each pair of molecules in said training set using a pre-defined structural similarity metric;

selecting one of said target molecules (T) ~~a target molecule from said first subset~~;

sorting all training set molecules in descending order of structural similarity to molecule T as defined by the computed numerical values;

defining, for a first one of said sorted training set molecules (M) ~~a first molecule in said training set other than said target molecule,~~ a fractions-correctly-predicted metric as a ratio of A/B, wherein B is defined as the total number of training set molecules that have a computed numerical structural similarity to molecule T that is as large or larger than the computed numerical structural similarity between molecules T and M, and wherein A is defined as the number of training set molecules that both (1) have a computed numerical structural similarity with molecule T that is as large or larger than the computed numerical

structural similarity between molecules T and M, and (2) possess the at least one chemical or biological property ~~as the number of molecules in said training set that are members of said first subset and that have a structural similarity to said target molecule at least as great as said first molecule's structural similarity to said target molecule divided by the total number of molecules in said training set having a structural similarity to said target molecule at least as great as said each other molecule's structural similarity to said target molecule~~;

repeating the defining step for ~~each molecule~~ other sorted training set molecules ~~in said training set other than said target molecule~~;

~~determining, from molecules in said training set having a fractions correctly predicted metric below a threshold value, which molecule has the highest structural similarity to said target molecule;~~

~~counting the number of molecules in said training set having a higher structural similarity to said target molecule than said molecule determined in said determining step;~~

choosing ~~said target molecule~~ molecule T as a marker molecule if said number B and said ratio A/B are both above respective threshold values when computed during at least one of said defining steps; ~~of molecules determined in the counting step is equal to or greater than a pre selected value~~; and

outputting data indicating that ~~said target molecule~~ molecule T has been chosen as a marker molecule.

4. (CANCELED)

5. (CANCELED)

6. (CURENTLY AMENDED) The method of Claim 3, additionally comprising repeating said ~~determining and counting steps~~ choosing for a plurality of different threshold values.

7. (CURRENTLY AMENDED) The method of Claim 3, comprising repeating said selecting a target molecule, sorting, defining, ~~repeating, determining, counting,~~ and choosing steps for other molecules ~~of said first subset~~ that possess the at least one chemical or biological

property at a plurality of different threshold values ~~and pre-selected number of molecules value~~ so as to select a plurality of preliminary sets of marker molecules.

8. (PREVIOUSLY PRESENTED) The method of Claim 7, comprising choosing a final set of marker molecules by making molecular behavior predictions for all molecules in said training set using each one of said preliminary sets of marker molecules, and choosing as said final set of marker molecules the preliminary set that most accurately predicts molecular behavior of molecules of said training set.

9-18. (CANCELED)

19. (NEW) The method of Claim 3, wherein said threshold for B is 5, and said threshold for A/B is 1.

SUMMARY OF INTERVIEW

Exhibits and/or Demonstrations

none

Identification of Claims Discussed

Claim 3

Identification of Prior Art Discussed

none

Proposed Amendments

none

Principal Arguments and Other Matters

The steps of the method were discussed. Applicant's representative explained the significance of the claim limitations in terms of producing predictive models for chemical behavior of molecules.